Free expansion of a Bose-Einstein condensate at the presence of a thermal cloud

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We investigate numerically the free-fall expansion of a ^{87}Rb atoms condensate at nonzero temperatures. The classical field approximation is used to separate the condensate and the thermal cloud during the expansion. We calculate the radial and axial widths of the expanding condensate and find clear evidence that the thermal component changes the dynamics of the condensate. Our results are confronted against the experimental data.

Since the first experimental realization of a Bose-Einstein condensation in dilute atomic gases [1] the measurement techniques based on time-of-flight expansion became a powerful method to study ultracold atomic systems. In fact, this kind of measurement was used to prove the existence of a condensate. Starting from an axially (cigar- or disc-shaped) symmetric atomic cloud it happened after its release from a trap that the ratio of the axial and radial both condensate and thermal cloud widths systematically change during the expansion. Eventually the anisotropy inversion for a condensate was observed which was a crucial distinction from the behavior of a thermal cloud. The thermal part, in agreement with the classical Maxwell distribution of velocities eventually takes a spherical shape. For a small condensate (like the very first rubidium condensate consisting of some 2000 atoms only) the anisotropy inversion is just a direct manifestation of the Heisenberg uncertainty principle - more spatial squeeze - higher momenta. For larger samples similar inversion is a result of the interaction energy stored anisotropically in the trapped condensate. It is worth adding that the free expansion technique was also used for degenerate fermionic gases, for instance to probe the superfluidity of strongly interacting atomic Fermi mixtures [2] or to measure the p-wave Feshbach resonances for fermionic atoms [3].

The main purpose of this work is to investigate an influence of a thermal cloud on the dynamics of an expanding condensate. If such an impact exists another question is whether it is restricted only to times just after the release or is it continued over the whole expansion time. Finally, it would be interesting to know how the influence during the expansion compares to the influence while the system is confined.

To investigate the mutual interaction between the condensed and thermal components during the expansion we employ the classical field approximation in a version described in Ref. [4]. So, we start with N-particle Hamiltonian written in terms of the field operator $\hat{\Psi}(\mathbf{r}, t)$ satisfying the bosonic commutation relations. Assuming the usual contact interaction potential for colliding atoms the Hamiltonian takes the form:

$$
\begin{aligned}
H = & \int d^3r \, \hat{\Psi}^+(\mathbf{r}, t) \left[-\frac{\hbar^2}{2m}\nabla^2 + V_{tr}(\mathbf{r}, t) \right] \hat{\Psi}(\mathbf{r}, t) \\
& + \frac{g}{2} \int d^3r \, \hat{\Psi}^+(\mathbf{r}, t)\hat{\Psi}^+(\mathbf{r}, t)\hat{\Psi}(\mathbf{r}, t)\hat{\Psi}(\mathbf{r}, t),
\end{aligned} \tag{1}
$$

where the interaction strength $g = 4\pi\hbar^2 a/m$ and a is the s-wave scattering length. The trapping potential $V_{tr}(\mathbf{r}, t)$ is time-dependent and is switched off instantaneously to trigger the expansion. The main equation of the classical field approximation reads:

$$
\begin{aligned}
i\hbar\frac{\partial}{\partial t}\Psi(\mathbf{r}, t) = & \left[-\frac{\hbar^2}{2m}\nabla^2 + V_{tr}(\mathbf{r}, t) \right] \Psi(\mathbf{r}, t) \\
& + g\,\Psi^*(\mathbf{r}, t)\Psi(\mathbf{r}, t)\Psi(\mathbf{r}, t)
\end{aligned} \tag{2}
$$

and is just the Heisenberg equation of motion for the field operator stripped of its operator character. The complex wave function $\Psi(\mathbf{r}, t)$ which we call the classical field describes both condensed and noncondensed atoms. The use of the classical field instead of the field operator is justified when only macroscopically occupied modes are taken into consideration. This reasoning remains in analogy with the treatment of an intense light beam which although consisting of single photons maybe described by the electric and magnetic fields.

An important question how to get out of the classical field the information on a condensate and a thermal cloud is resolved by using of Penrose and Onsager definition of a Bose-Einstein condensation [5] and by taking into consideration a measurement process. Since any detector has a limited spatial and temporal resolutions a complicated (both in space and time) behavior of the high energy classical field is smoothed out during the measurement. Therefore, the quantity which is physically important is a time and/or space averaged one-particle density matrix. According to the Penrose and Onsager definition the condensate wave function is an eigenvector corresponding to the dominant eigenvalue of a one-particle coarse-grained (i.e., averaged over time and/or space) density matrix. We closely follow the experiment and realize the averaging as a column integration along one of the radial directions. The physically important (averaged along y

direction) one-particle density matrix is given by

$$\bar{\rho}(x, z, x', z'; t) = \int dy\, \Psi(x, y, z, t)\, \Psi^*(x', y, z', t) \quad (3)$$

and the splitting procedure requires the diagonalization of (3). This kind of averaging was already used to investigate a decay of multiply charged vortices [6]. The splitting procedure is then summarized as:

$$\bar{\rho} = \sum_k N_k\, \varphi_k(x, z, t)\, \varphi_k^*(x', z', t) \quad (4)$$

$$\psi_0(x, z, t) = \sqrt{N_0}\, \varphi_0(x, z, t) \quad (5)$$

$$\rho_T(x, z, t) = \bar{\rho}(x, z, x, z; t) - |\psi_0(x, z, t)|^2. \quad (6)$$

Here, φ_k are the macroscopically occupied modes, N_0 is the dominant eigenvalue, ψ_0 is the condensate wave function, and ρ_T is the density of thermal cloud.

Having introduced the classical field approximation we now describe our numerical procedure. First, we find the classical field corresponding to the ^{87}Rb Bose gas (with a scattering length $a = 5.82\,\text{nm}$) at equilibrium confined in a harmonic trap with frequencies $\omega_\perp \equiv \omega_{x,y} = 2\pi \times 137.4\,\text{Hz}$ and $\omega_z = 2\pi \times 12.6\,\text{Hz}$. Details on how to obtain an equilibrium state for a given number of atoms and at particular temperature are explained elsewhere [7]. Since we intend to investigate the influence of thermal atoms on the condensate expansion we prepare various equilibrium states but we keep the same number of condensed atoms (30000 or 90000) in all of these states. Next, we suddenly turn off the trapping potential and let the atomic cloud to expand. Technically speaking, we solve the Eq. (2) on a larger grid (but having the same spatial step) and without any trap. We monitor the momentum distribution (i.e., the Fourier transform of the classical field) during the expansion and find that it changes for the first few milliseconds only. In other words, a few milliseconds is required to convert fully the interaction energy into the kinetic energy. Afterwords, the classical field evolves freely and can be found with the help of the propagator of the free Schrödinger equation. Finally, at a desired time the splitting of the classical field into the condensed and noncondensed components is performed.

In Fig. 1 we plot the radial and axial densities of an expanding atomic cloud at 22 ms. Initially the condensate is a cigar-shaped like a trap. Its aspect ratio in the Thomas-Fermi approximation is given by $R_\perp/R_z = \omega_z/\omega_\perp$ [8] which equals approximately 1/10. After 22 ms, as can be seen in Fig. 1, the initial anisotropy is, actually, inverted. The radial size gets larger than the axial one. This, of course, is not true for the thermal cloud in which case the final density becomes spherical.

Fig. 2 reveals some technical details related to the read-out procedure. After the splitting of the classical field is concluded and the two-dimensional condensate density is known, this density is fitted by a two-dimensional inverted parabola (since according to the
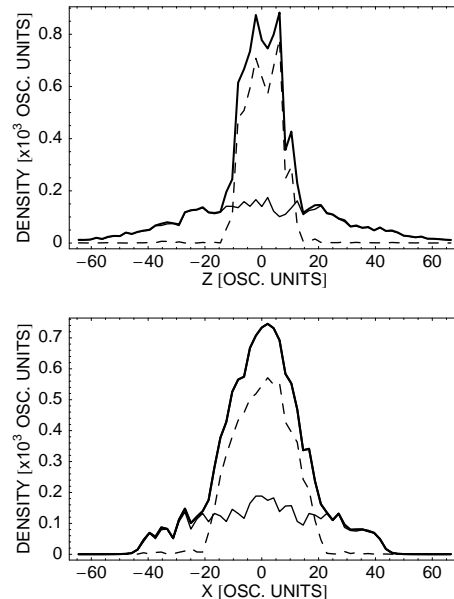

FIG. 1: Axial (upper frame) and radial (lower frame) cuts of the total (thick solid line), condensate (dashed line), and thermal (thin solid line) densities as obtained by splitting the free expanding classical field at 22 ms as described in the text. The condensate fraction is equal to 0.3 and the number of condensed atoms $N_0 = 90000$. The oscillatory unit of length is defined based on the axial trap frequency: $\sqrt{\frac{\hbar}{m\omega_z}}$ and equals $3.0\,\mu m$.

large number of atoms in the condensate the Thomas-Fermi approximation is valid). The fit is performed based on the least squares method. In fact, fits depend on the realization and, as will be shown later, the aspect ratio is a quantity which is most sensitive to the realization.

The main result of this work is presented in Fig. 3. It shows the radial and axial condensate widths after 22 ms of free expansion as a function of a condensate fraction. There are two sets of data included in this figure. The first one (squares and circles) depicts the behavior of the system with the same number of condensed atoms ($N_0 = 90000$) independently of the condensate fraction (i.e., temperature). The second set (starts and triangles) represents data for the systems with $N_0 = 30000$. Horizontal lines are the radial and axial sizes of 9×10^4 and 3×10^4 atoms condensate calculated within the expansion model formulated by Castin and Dum [9]. This model describes the free expansion of a pure condensate within the Thomas-Fermi limit. Our data suggest that thermal atoms somehow temper the expansion of the condensate.

There are three experimental papers discussing the temperature effects having influence on the ballistic expansion of a condensate [10, 11, 12]. All of these papers claim that the behavior of the condensed cloud measured in terms of its size during the expansion depends on the temperature of the system before the expansion. So, the quantitative comparison between the numerical calcula-
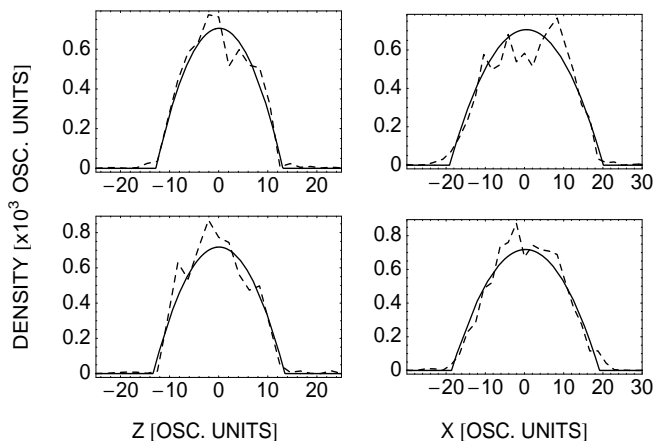
FIG. 2: Condensate axial (left frame, dashed line) and radial (right frame, dashed line) densities for two single realizations (upper and lower frames, respectively) at 22 ms. Condensate density is extracted from the classical field by the splitting procedure and is fitted to two-dimensional inverse parabola. Black lines show axial (left frame) and radial (right frame) cuts of such a fit. The parameters are the same as in Fig. 1.
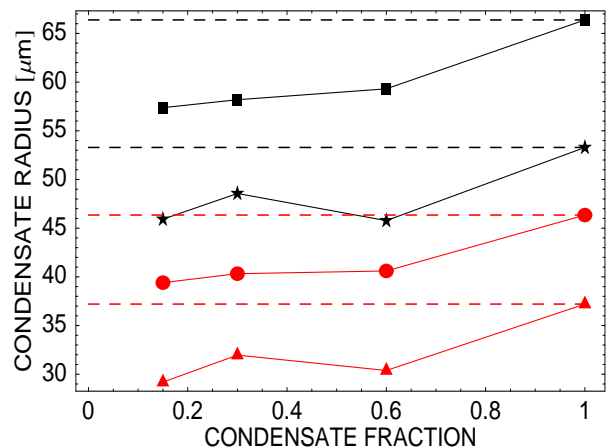

FIG. 3: (Color online) Radial (squares and stars) and axial (circles and triangles) condensate radii as a function of the condensate fraction after 22 ms of ballistic expansion. Two sets of points marked by squares and circles correspond to the systems with the number of condensed atoms $N_0 = 90000$ whereas two other sets (marked by stars and triangles) represent the systems with $N_0 = 30000$ condensed atoms. Solid lines are shown to guide the eye. Horizontal dashed lines are the Thomas-Fermi values for the radial lengths (two upper lines, the upper line for $N_0 = 90000$ and the lower line for $N_0 = 30000$) and the axial lengths (two lower lines, the upper line for $N_0 = 90000$ and the lower line for $N_0 = 30000$). Note that both radial and axial widths get shorter in comparison with the size of a pure condensate of the same number of atoms.

tions and the experiment is possible.

Since our numerical parameters were taken in a way to match the parameters of experiment of Ref. [11] we start with this paper. In that experiment the authors make effort to keep constant the number of condensed atoms while expanding the atomic samples at various temperatures. They found the increase of radial and axial condensates lengths when the temperature gets higher (see Fig. 4 in [11]). The measured widths are larger than the corresponding Castin-Dum values. So, the authors claim that their experiment is performed in the non-Thomas-Fermi regime. An increase of radial and axial widths with temperature is explained by an assumption that at equilibrium in a trap the thermal atoms exert a force on condensed atoms towards the center of a trap thus compressing the condensate cloud. This compression results in a faster expansion in all directions after the trap is released. However, our calculations within the classical field approximation show that, actually, no compression of a condensate cloud occurs in a trap. We stress that this statement is true also within the self-consistent Hartree-Fock model [8]. In Fig. 4 we plot axial and radial condensate densities obtained by solving selfconsistently the equations of the Hartree-Fock model for a particular number of condensed atoms ($N_0 = 90000$) but at various temperatures (solid lines which correspond to the condensate fractions 0.15, 0.30, and 0.60). We also added to the figure the densities of a pure condensate consisting of 90000 atoms calculated by solving the Gross-Pitaevskii equation in imaginary time (dotted line) as well as by the Thomas-Fermi formula (dashed line). Clearly, Fig. 4 shows no compression due to the presence of a thermal cloud.

A qualitative difference between numerical results and

the experimental data of Ref. [11] motivated us to make a comparison with other experimental works. For example, in Ref. [10] a deviation from ballistic expansion is also reported. In Fig. 5a of that paper the authors plot the aspect ratio of the condensed component after 22.3 ms of free expansion as a function of reduced temperature. It is clear from this figure that for higher temperatures the results are different than the Castin-Dum limit [9] (the aspect ratio shows deviation from the Castin-Dum values also in [11]). Therefore, we look separately at the axial and radial sizes of the expanding condensate in the case of Orsay experiment. The results are presented in Fig. 5. Here, the experimental data are compared with the Castin-Dum values. This figure clearly shows that the experimental data stay close to the Castin-Dum values. In axial direction the thermal cloud seems to temper the expansion of a condensate whereas the interplay between the condensate and the thermal component in radial direction gets more complicated. Differences are on the level of a few percent similarly to what we obtain from our numerics (although for a different trap geometry) and in opposite to what is reported in paper [11].

In other experimental work, Ref. [12], the authors find finite temperature correction to the Thomas-Fermi approximation as a function of the condensate fraction by measuring the ratio $\bar{R}^5/N_0$, where $\bar{R}$ is the condensate radius defined as $\bar{R} = (R_\perp^2 R_z)^{1/3}$ and N_0 is the num-
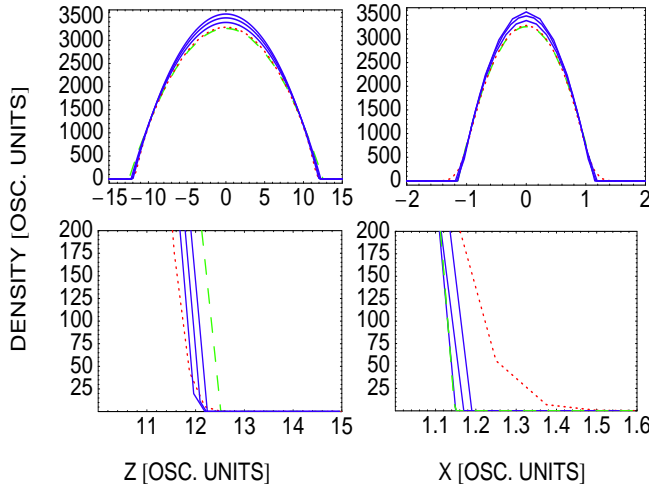
FIG. 4: (Color online) Axial (left frames) and radial (right frames) condensate density cuts for a system with $N_0 = 90000$ condensed atoms calculated within the self-consistent Hartree-Fock model (solid lines corresponding to the condensate fractions 0.15, 0.30, and 0.60), by the Gross-Pitaevskii equation (dotted line), and from the Thomas-Fermi formula (dashed line). Lower panel shows in detail the region the density drops to zero.

ber of condensed atoms. There is an agreement with Castin-Dum predictions [9] for low temperatures, however, when the temperature gets higher the ratio $\bar{R}^5/N_0$ departs from the Castin-Dum value getting larger (see Fig. 4 of [12]). The authors explain this behavior by using a combination of a modified Hartree-Fock model to describe the condensed and thermal fractions in a trap and an expansion model formulated by Castin and Dum [9]. They conclude that the influence of the thermal cloud on the condensate during the expansion is negligible which seems to be in opposition to what is claimed in Refs. [10] and [11]. It contradicts also our findings. Therefore, we decided to compare all experiments and our numerical results on a graph where we plot $\bar{R}^5/N_0$ (actually, normalized to the value given by the Castin-Dum approach to make the comparison feasible) as a function of the condensate fraction. In Castin-Dum formulation one has

$$\bar{R}^5(t)/N_0 = 15\, a\, \bar{a}^4 (\lambda_\perp^2(t)\, \lambda_z(t))^{5/3} \qquad (7)$$

where

$$\lambda_\perp(t) = \sqrt{1 + t^2}$$
$$\lambda_z(t) = 1 + \beta^2(t \arctan t - \ln\sqrt{1 + t^2}), \qquad (8)$$

$\beta = \omega_z/\omega_\perp$ and time t is expressed in units of $1/\omega_\perp$ whereas $\bar{a}$ is an oscillatory unit length calculated based on the geometric mean of all angular frequencies. Fig. 6 shows that our results (solid squares for $N_0 = 90000$ and open squares for $N_0 = 30000$) stay in a quite good agreement with Orsay experimental data.
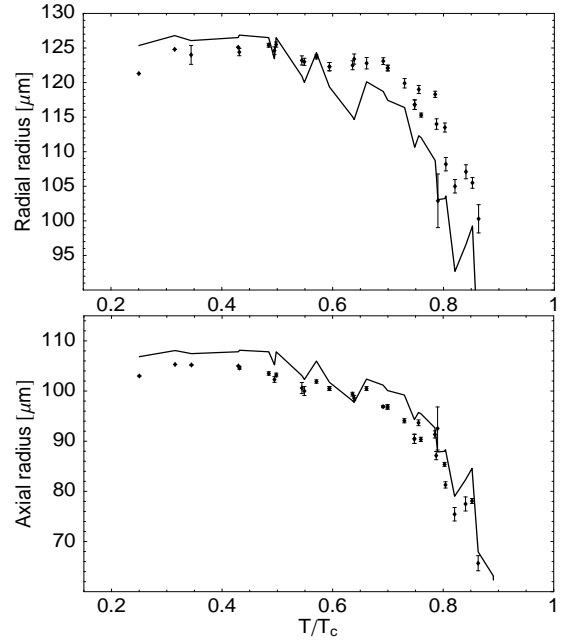

FIG. 5: Radial (upper panel) and axial (lower panel) widths as a function of reduced temperature. Experimental data (points with error bars) correspond to the experiment of Ref. [10] whereas numerical results (solid lines) are calculated based on the Castin-Dum approximation.

Certainly, further experimental and theoretical effort is required to gain more insight to what, indeed, is happening during the expansion of condensate and thermal cloud.

Finally, in Fig. 7 we plot the aspect ratio for a condensate for various condensate fractions. The aspect ratio seems to be a quantity which is most sensitive to the interplay between the thermal cloud and the condensate. For low temperatures the aspect ratio approaches the Castin-Dum value whereas for higher temperatures it is getting larger. Moreover, we find that the aspect ratio is very sensitive to the initial conditions fulfilled by the classical field. Different realizations lead to different aspect ratios what is marked by error bars in Fig. 7.

In conclusion, we have studied the expansion of the Bose-Einstein condensate at the presence of thermal atoms. Using the classical field approximation we have shown that thermal atoms change the dynamics of a condensate in a way that both radial and axial condensate widths get smaller in comparison with the case when there is no thermal cloud. It results in a change of condensate aspect ratio which becomes bigger for smaller condensate fraction (i.e., larger thermal cloud). While all papers agree that the thermal cloud does play a role in the expansion of the condensate, the details remain unclear. The three experimental papers are not mutually in agreement and also our results do not coincide with some measurements. Clearly more work is needed to clarify this somewhat confusing situation.
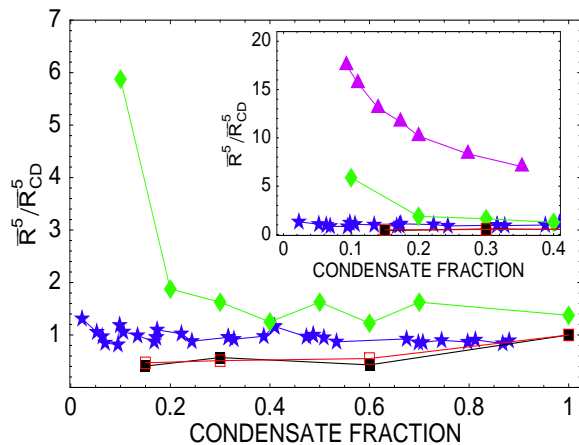
FIG. 6: (Color online) Ratio $\bar{R}^5/N_0$ (normalized to the value obtained from the Castin-Dum approximation) as a function of the condensate fraction. The mean size of the condensate is defined as $\bar{R} = (R_\perp^2 R_z)^{1/3}$. Four sets of data are presented in the figure according to the numerical calculations (solid and open squares), the results of Ref. [10] (stars), Ref. [12] (diamonds), and Ref. [11] (inset, triangles).
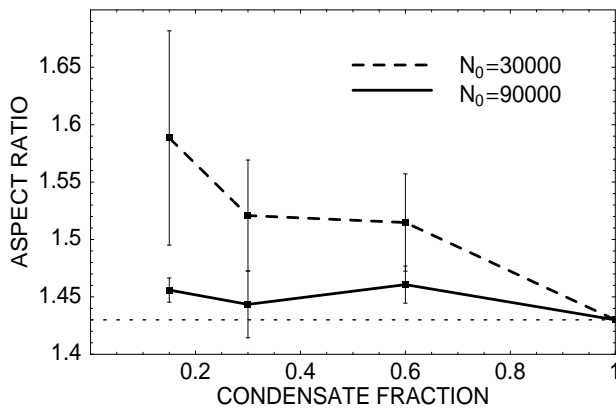

FIG. 7: Aspect ratio $(R_\perp/R_z)$ at $22\,\mathrm{ms}$ defined as the ratio of radial and axial condensate widths for various condensate fractions. Two sets of data are presented corresponding to the number of condensed atoms $N_0 = 90000$ (solid line) and $N_0 = 30000$ (dashed line). Error bars depict the dependence on the realization. Horizontal dashed (thin) line is the aspect ratio obtained within the Thomas-Fermi approximation.

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